

Modeling and Uncertainty Quantification of Thermoelastic Damping in Micro-Resonators

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ABSTRACT

In the design of micro-electromechanical systems (MEMS) such as micro-resonators, dissipation mechanisms may have detrimental effects on the quality factor, which is directly related to the response amplitude of the system that is excited at its natural frequency. One of the major dissipation phenomena to be considered in such micro-systems is thermoelastic damping. Hence, the performance of such MEMS is directly related to their thermoelastic quality factor which has to be predicted accurately.

Moreover, the performance of MEMS depends on manufacturing processes which may cause substantial uncertainty in the geometry and in the material properties of the device. The reliability of MEMS devices is affected by the inability to accurately predict the behavior of the system due to the presence of these uncertainties. The aim of this paper is to provide a framework to account for uncertainties in the finite element analysis. Particularly, the influence of uncertainties on the performance of a micro-beam is studied using Monte-Carlo simulations. A random field approach is used to characterize the variation of the material as well as the geometric properties. Their effects on the thermoelastic quality factor of a micro-beam are studied.

Nomenclature

b	Influence length
C	Damping matrix
F	Force vector
H	Random field
K	Stiffness matrix
L	Length of the random field domain
M	Mass matrix
λ	Eigenvalue
μ	Mean
ρ	Correlation function
σ	Standard deviation
τ	Lag
ω	Pulsation

Introduction

The performance of a micro-electromechanical system can vary because of uncertainties. Manufacturing processes may leave substantial uncertainty in the shape and geometry of the device while the material properties of a component are inherently subject to scattering. The design of accurate MEMS has to take into account the influence of these uncertainties. In the literature, different works were carried out to quantify the effect of the uncertainties on electrostatically actuated MEMS [1-4]. These studies considered the material and

geometric parameters as random variables and used Monte-Carlo methods as well as first and second order reliability methods.

In this paper, the effects of uncertainties on micro-resonators are studied. For this kind of MEMS, dissipation mechanisms may have detrimental effects on their performance which is quantified by their quality factor. One of the major dissipation phenomena to consider is thermoelastic damping [5-6]. Hence, in order to quantify the effects of the uncertainties on the performance of micro-resonators, the variation of the thermoelastic quality factor is studied. In the present paper, the thermoelastic quality factor of a micro-beam is studied as an example. Monte-Carlo simulations are carried out in order to determine the mean and the coefficient of variation of the thermoelastic quality factor. In these simulations, the elasticity modulus is modeled as a random field and the length of the beam as a random variable.

The paper is organized as follows. Firstly, the procedure to quantify the thermoelastic quality factor is exposed. An efficient thermoelastic finite element formulation is the key point in order to investigate the influence of uncertainties on the behavior of micro-systems. Then, different methods to generate random fields are discussed. Finally, the results of Monte-Carlo simulations are presented.

Thermoelastic Damping

Thermoelastic damping represents the loss in energy from an entropy rise caused by the coupling between heat transfer and strain rate. Analytical models exist for simple configurations such as beams [7-8]. However, a numerical approach is required in order to take into account the spatial variation of the material properties. A thermoelastic finite element formulation was derived in [9] and showed efficiency in order to estimate the thermoelastic quality factor.

The thermoelastic finite element formulation can be derived from Hamilton's variational principle in which both mechanical and thermal degrees of freedom are considered simultaneously. The displacement field \mathbf{u} and the temperature increment θ are related by the dynamic equilibrium equation governing the thermoelastic problem

$$\begin{pmatrix} M_{uu} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \ddot{u}_u \\ \ddot{u}_\theta \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ C_{\theta u} & C_{\theta\theta} \end{pmatrix} \begin{pmatrix} \dot{u}_u \\ \dot{u}_\theta \end{pmatrix} + \begin{pmatrix} K_{uu} & K_{u\theta} \\ 0 & K_{\theta\theta} \end{pmatrix} \begin{pmatrix} u_u \\ u_\theta \end{pmatrix} = \begin{pmatrix} F_u \\ F_\theta \end{pmatrix} \quad (1)$$

where M_{uu} is the mass matrix, $C_{\theta u}$ is the damping matrix due to the thermo-mechanical coupling effect and $C_{\theta\theta}$ is the damping matrix due to the thermal field. The matrix $K_{u\theta}$ is the stiffness matrix due to the thermo-mechanical coupling. Matrices K_{uu} and $K_{\theta\theta}$ are the stiffness matrices due to mechanical and thermal fields, respectively. Vectors F_u and F_θ are the excitation force vectors associated to mechanical and thermal fields, respectively.

In order to determine the thermoelastic quality factor, the thermoelastic frequencies have to be computed. The eigenvalue problem corresponding to the thermoelastic problem (eq. 1) is:

$$\begin{pmatrix} -K_{uu} & -K_{u\theta} & 0 \\ 0 & -K_{\theta\theta} & 0 \\ 0 & 0 & M_{uu} \end{pmatrix} \begin{pmatrix} x_u \\ x_\theta \\ \dot{x}_u \end{pmatrix} = \lambda \begin{pmatrix} 0 & 0 & M_{uu} \\ C_{\theta u} & C_{\theta\theta} & 0 \\ M_{uu} & 0 & 0 \end{pmatrix} \begin{pmatrix} x_u \\ x_\theta \\ \dot{x}_u \end{pmatrix} \quad (2)$$

If the number of mechanical and thermal degrees of freedom is denoted by n_u and n_θ , respectively, the eigenvalue problem (eq. 2) has $2 n_u$ conjugate complex eigenvalues and n_θ real eigenvalues. The $2 n_u$ eigenvalues correspond to the mechanical frequencies and the n_θ ones to the thermal frequencies. Hence the quality factor of the n th mode is given by

$$Q = \frac{\omega_r}{2\omega_i} \quad (3)$$

where ω_r and ω_i are the real and imaginary parts of the n th conjugate complex eigenvalue of equation (2).

Random Field Discretization Methods

The aim of this section is to provide a framework to account for uncertainties in the finite element analyses. A random field approach has to be used to characterize the spatial variation of the material properties. Vanmarcke [10] provides extensive details on the analysis and synthesis of random fields. In order to discretize a random

field, i.e. to represent a random field with a finite set of random variables, different methods are available in the literature [11]. In this work, two different methods are investigated: the Local Average method and the Karhunen-Loeve expansion. These methods are used to discretize 1-D random fields. These fields are assumed to be Gaussian and homogeneous so that they are fully characterized by the mean μ , the standard deviation σ and the correlation function $\rho(\tau)$ where τ is the lag vector. In this work, the exponential correlation function is used:

$$\rho(\tau) = e^{-\frac{|\tau|}{b}} \quad (4)$$

where b is the influence length.

The Local Average method is an average discretization method, i.e. the random variables are defined as weighted integrals of the random field over a domain. Hence, the random field discretization requires the definition of a mesh, which in this work, is chosen to be the finite element mesh. The number of random variables corresponds to the number of elements. The Local Average method, which consists in approximating the field in each element as a constant being computed as the average of the original field over the element, was suggested by Vanmarcke [10]. The covariance matrix can be calculated using expressions that have been derived for homogeneous fields [10]

For 1-D random field, the covariance between two elements U and U' is given by:

$$Cov(U, U') = \frac{\sigma^2}{2UU'} [U_0^2 \gamma(U_0) - U_1^2 \gamma(U_1) + U_2^2 \gamma(U_2) - U_3^2 \gamma(U_3)] \quad (5)$$

where $\gamma(x)$ is the variance function corresponding to the correlation function and U_0, U_1, U_2 and U_3 are distances as illustrated in figure 1.

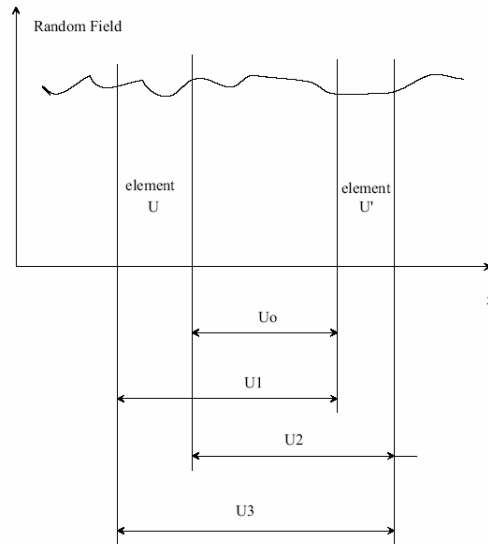


Figure 1 – Definition of distances in expression for covariance between local averages

The domain is divided into equal elements. Non-equal elements can be used but they may lead to a non-positive covariance matrix. The random field is generated in three basic steps:

- A random uncorrelated Gaussian vector Z , whose size is equal to the number of elements, is generated.
- The covariance matrix is obtained from equation (5).
- The correlated vector X is obtained by Cholesky transformation: $X = L Z$ where L is a lower triangular matrix obtained by the Cholesky decomposition of the covariance matrix, which is definite positive.

The Karhunen-Loeve expansion [12] is a series expansion method where the field is represented as a truncated series involving random variables and deterministic spatial functions. Karhunen-Loeve expansion of a field $H(x, \xi)$ is based on the spectral decomposition of the covariance function and is given by:

$$H(x, \xi) = \mu + \sum_{k=1}^N \sqrt{\lambda_k} f_k(x) b_k(\xi) \quad (6)$$

where $b_k(\xi)$ is the k th random variable, the eigenvalues λ_k and eigenfunctions $f_k(x)$ of the covariance kernel can be calculated analytically for an exponential correlation function. Note that the dependency on ξ in $H(x, \xi)$ and $b_k(\xi)$ underlines the random nature of the field H and the variable b_k . For 1-D random fields on a domain $[0, L]$, the eigenvalues are given by [12]:

$$\lambda_k = \frac{2\sigma^2 b}{1 + b^2 \omega_k} \quad (7)$$

where ω_k is the k th root of the following transcendental functions:

$$f(\omega) = \omega - \frac{\cos(\omega L) - 1}{b \sin(\omega L)} \text{ for } k \text{ even} \quad (8)$$

and

$$f(\omega) = \omega - \frac{\cos(\omega L) + 1}{b \sin(\omega L)} \text{ for } k \text{ odd} \quad (9)$$

Similarly, the eigenfunctions are expressed as function of ω_k :

$$f_k(x) = \sqrt{\frac{2\omega_k}{\omega_k L - \sin(\omega_k L)}} \sin\left(\omega_k \left(x - \frac{L}{2}\right)\right) \text{ for } k \text{ even} \quad (10)$$

and

$$f_k(x) = \sqrt{\frac{2\omega_k}{\omega_k L + \sin(\omega_k L)}} \cos\left(\omega_k \left(x - \frac{L}{2}\right)\right) \text{ for } k \text{ odd} \quad (11)$$

In series expansion method, such as Karhunen-Loeve expansion, the approximation is introduced by the truncation of the sum in equation (6). N is the order of expansion, which is also the number of random variables.

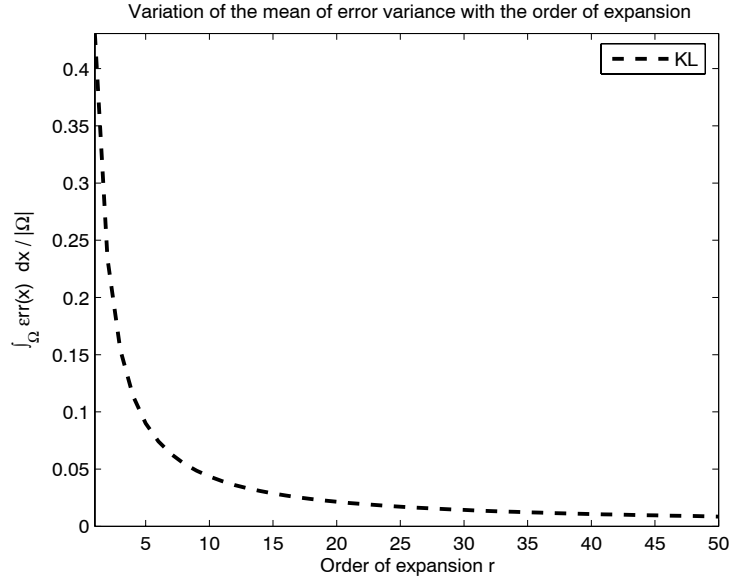


Figure 2 – Variation of the error on the variance with the order of expansion

Figure 2 shows the evolution of the mean of the variance error as a function of the order of expansion. When the order of expansion is larger than eight, the mean of the error variance is less than 5 %. The order of expansion is set to 10 in this work.

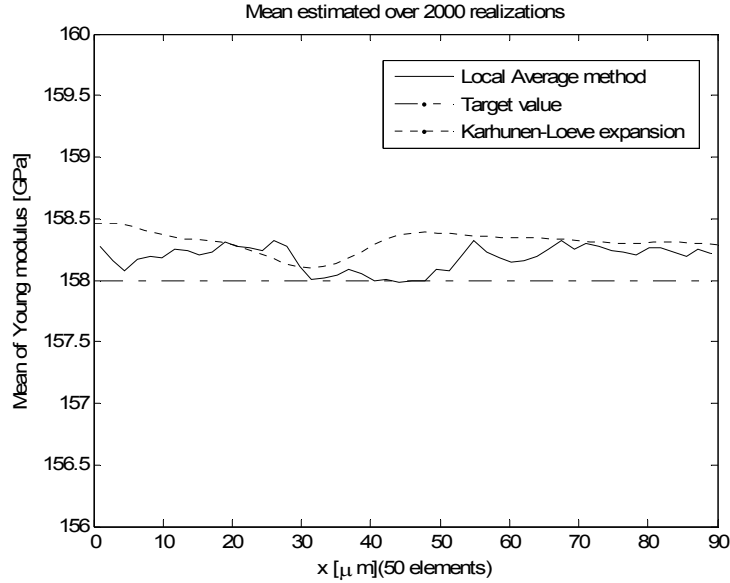


Figure 3 – Random field mean of 2000 realizations

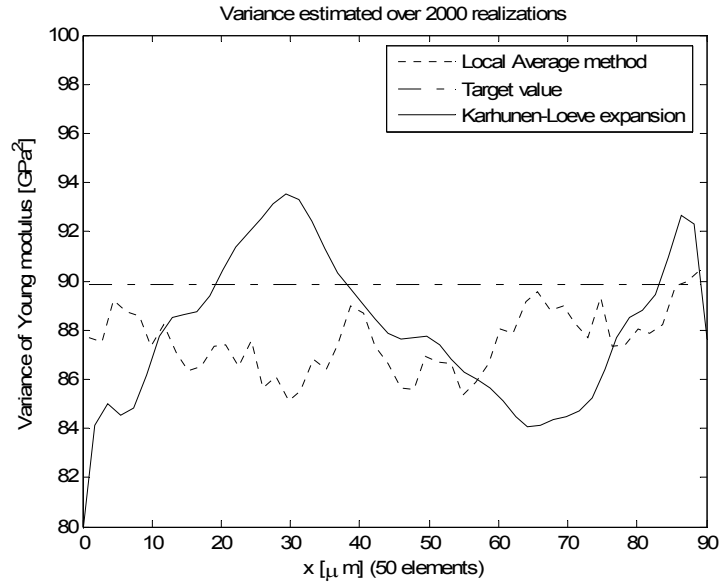


Figure 4 – Random field variance of 2000 realizations

Random Field Generation

The Local Average method and the Karhunen-Loeve expansion are used in order to model the spatial variation of the elasticity modulus of a silicon beam whose dimensions are $90 \mu\text{m} \times 4.5 \mu\text{m} \times 4.5 \mu\text{m}$. For both methods, 2000 sample random fields are generated, which are used to carry out Monte-Carlo simulations of the thermoelastic quality factor of the beam in next section. The mean and the coefficient of variation are set to 158 GPa and 6%, respectively, which correspond to values of silicon thin films [13]. The coefficient of variation of 6% is equivalent to a variance of 90 GPa^2 . The influence length b is set to an arbitrary value of $45 \mu\text{m}$, which is half the beam length.

For the Local Average method, the mesh consists in 50 equal elements as the finite element mesh and for the Karhunen-Loeve expansion, the random fields are estimated on the middle point of each element.

Figures 3 and 4 represent the spatial variation along the beam of the mean and the variance, respectively, of the 2000 samples. With 2000 realizations, the mean error is below 0.5 % for both methods. Concerning the variance, the error is less than 5% for the Local Average method but for the Karhunen-Loeve expansion, the error is larger at the boundaries of the domain. Indeed, on the left hand side of the beam, the error reaches its larger value which is 10 %. The mean of the variance error along the beam is less than 5 % as the order of expansion is larger than 8 (Figure 2). The divergence of the error at the boundaries of the random field is characteristic of the series expansion methods and their inherent truncation.

Figure 5(a) shows the covariance function of the 2000 random field realizations estimated at $x=0$. The covariance functions are similar to the exponential function for both methods. The covariance at the origin is equal to the variance. As the covariance is estimated at one boundary of the beam, the Karhunen-Loeve curve is different to the other curves near the origin. This difference is due to the divergence of the variance at the boundaries for series expansion methods. Figure 5(b) shows that the covariance matrix for the Karhunen-Loeve expansion is similar to exact covariance function except at the boundaries.

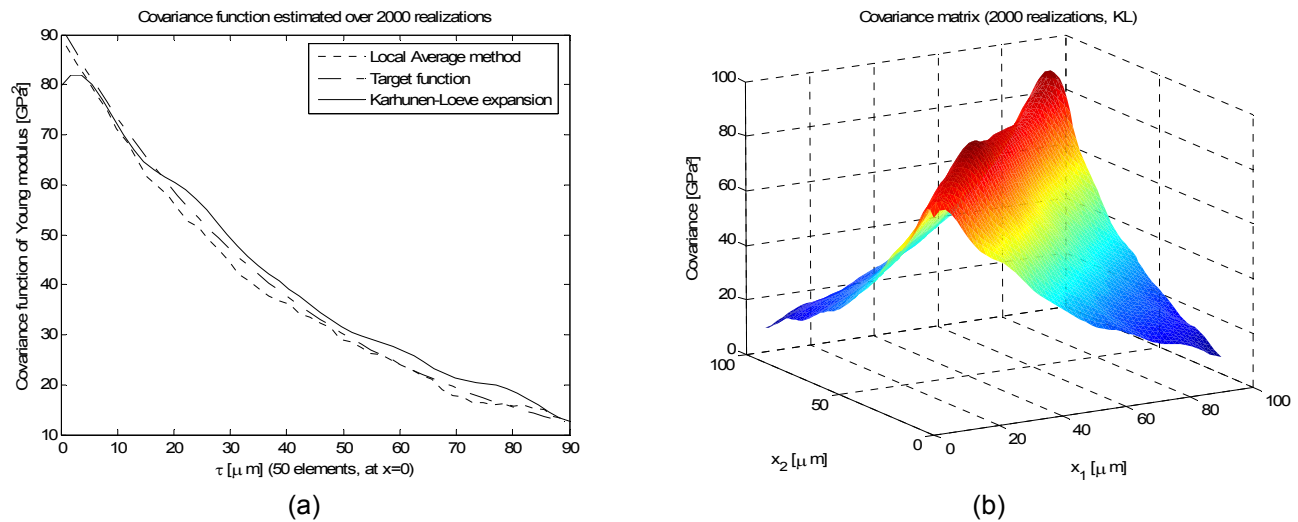


Figure 5 – Covariance of the elasticity modulus estimated over 2000 realizations

Monte Carlo Simulations

Direct Monte-Carlo simulations are carried out in order to quantify the influence of uncertainties on the thermoelastic quality factor of MEMS. The mean and the standard deviation of the quality factor can be obtained in four basic steps:

- A realization is generated of the structure whose material and/or geometric properties vary according to the given statistical law using a random field discretization method to take into account the spatial variation.
- The finite element method is used to calculate the quality factor for this realization.
- Steps 1-2 are repeated to obtain different statistical samples of the quality factor.
- The mean and variance of the quality factor samples are computed using appropriate averaging of the samples.

In the simulation procedure (step 1), material properties are generated at a specified number of points. For the finite element method, material properties need to be specified for each element. In the Local Average method, the random field mesh is the same as the finite element mesh and the material properties is specified for each element. For the Karhunen-Loeve expansion, for each finite element, material properties are set to the value of the random field (generated by the KL expansion) at the middle point of the element.

The proposed method is illustrated by numerical studies on the clamped-clamped silicon beam of $90\text{ }\mu\text{m} \times 4.5\text{ }\mu\text{m} \times 4.5\text{ }\mu\text{m}$. This structure is modeled with 50 equal thermoelastic beam elements. The deterministic thermoelastic quality factor of the first flexural mode of this beam is equal to 15 218.

Two simulations are considered. Firstly, the length of the beam is considered as a random variable. Then the Young modulus is considered as a random field with a mean of 158 GPa and a coefficient of variation of 6%. In both cases, an exponential correlation function with a correlation length of $45\text{ }\mu\text{m}$ is used to illustrate the methods. Two different discretization methods are used: the Local Average method and the Karhunen-Loeve expansion. In each case, 2000 simulations are carried out.

1. Length Variation

The length of the beam is considered to be random. It is modeled as a random variable with a normal density distribution. The mean and the coefficient of variation are set to $90\text{ }\mu\text{m}$ and 5 %, respectively. For each length, the finite element mesh consists in 50 equal beam elements. The maximum value of the length is $104\text{ }\mu\text{m}$ and the minimum one is $76\text{ }\mu\text{m}$. The mean of the samples is $90.0055\text{ }\mu\text{m}$ and their coefficient of variation is 4.95 %. Hence, the precision is of $10^{-3}\text{ }\%$ for the mean and 1 % for the coefficient of variation, which is satisfactory. The mean of the quality factor is equal to 15 381 and its coefficient of variation is 14.59 %. The mean of the quality factor is different from the deterministic value. This difference can be explained by the fact that the quality factor is not a linear function of the beam length as shown in figure 6. Due to this non-linear variation, the probability density function of the quality factor is not strictly Gaussian as shown in figure 7.

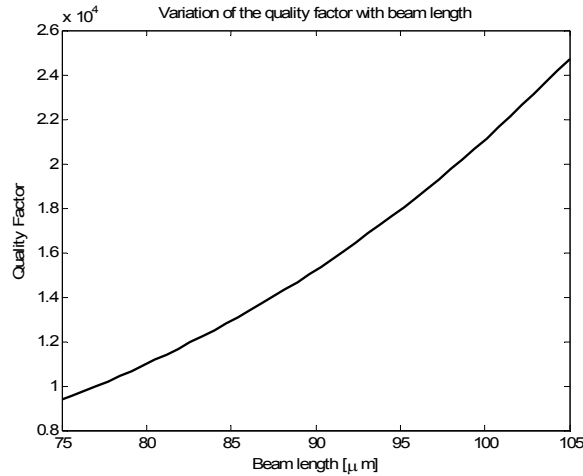


Figure 6 – Variation of the quality factor with beam length

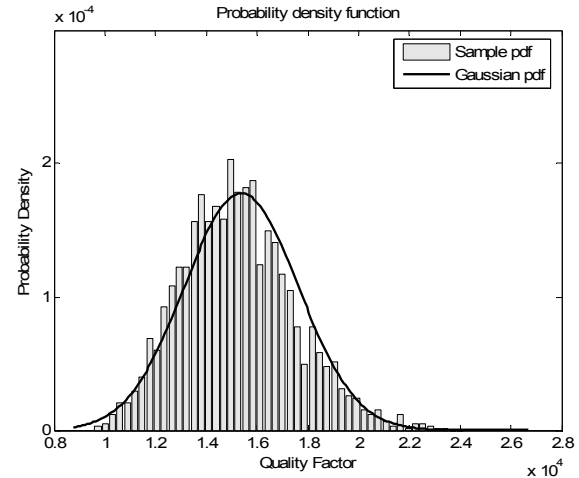


Figure 7 – Probability density function of the quality factor

2. Elasticity Modulus Variation

The uncertainties on Young's modulus are considered. Random field models are used to characterize the spatial variation of Young's modulus. Random fields whose properties are given in figures 3-5 are used for the Monte-Carlo simulations. The minimum and maximum values of the random fields are 118 GPa and 196 GPa. For the Local Average method, the mean of the quality factor is 15 249 and its coefficient of variation is 5.42%. For the Karhunen-Loeve expansion, the results are similar, i.e. 15 226 and 5.58%.

The coefficient of variation is slightly larger for the Karhunen-Loeve model because of the larger error on the variance of the generated random fields (Figure 4). The obtained quality factor means are larger than the quality factor of the determinist case. This is due to the fact that the quality factor is a non-linear function of the elasticity modulus as shown in figure 8. Due to this non-linear variation, the probability density function of the quality factor is not strictly Gaussian as shown in figure 9. Note that with the results shown in figure 3, the generated random fields overestimate the mean of the elasticity modulus what would underestimate the quality factor mean if the function was linear.

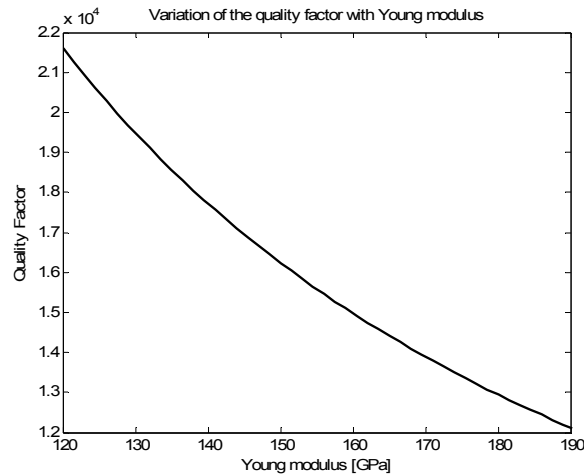


Figure 8 – Variation of the quality factor with Young's modulus

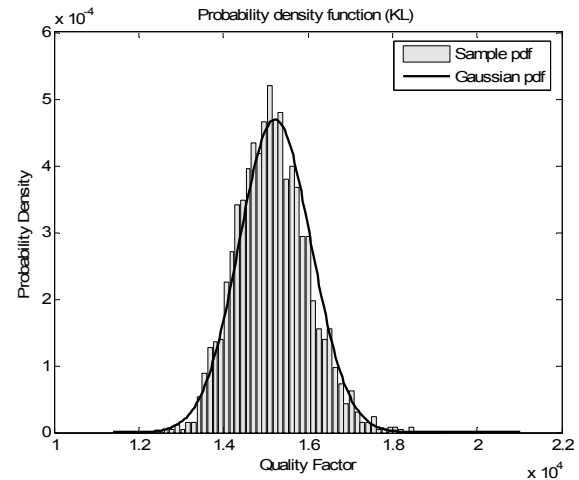


Figure 9 – Probability density function of the quality factor

It should be noted that the correlation length has been set arbitrarily to 45 μm . If this value is increased, the coefficient of variation increased and inversely. A change in the correlation length does not influence the mean of the quality factor in this case. In order to have a good estimation of the correlation length, micromechanics studies should be carried out on silicon thin film.

Conclusion

The principal objective of this study was to explore how numerical simulations can predict the variability in the performance of MEMS devices due to uncertainties. A computational framework has been presented for the analysis of the thermoelastic damping of MEMS under uncertainties. In order to model the spatial variation of the properties, random fields have been used. Direct Monte Carlo simulations have been carried out in order to quantify the mean and variance of the thermoelastic quality factor. In the present study, the proposed method has been illustrated on a simple numerical example. However, the method could be used in more complex problems. Several random variables and random fields (cross-related or not) could also be considered in order to take into account the uncertainties on several different parameters.

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